

201-14899B1

Methylhexahydrophthalic Anhydride (MHHPA)

2. PHYSICAL-CHEMICAL DATA

***2.2 BOILING POINT**

(a) Preferred result (score = 1)

Value: 299 degrees C

Remark: Measured at 99.02 kPa, by differential scanning calorimetry, using ASTM E537-86, Method 103 of the OECD Guidelines for Testing of Chemicals, 27 July 1995.

Reference: Methylhexahydrophthalic Anhydride (MHHPA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories
Project Number: 1592/003, 29 May, 2002

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*2.4 VAPOUR PRESSURE

(a) Preferred result (score = 2)

Value: 9.41 E-4

Temperature: 20 degree C

Test substances: MHHPA

Remark: Calculated using the Pitzer method

Remark:

Temperature degree C	mm Hg
20	0.000941
30	0.002645
40	0.006915
50	0.016704
60	0.038337
70	0.084223
80	0.174933
90	0.335973
100	0.689942
110	1.29431
120	2.322442
130	4.018134
140	6.931576
150	11.03331
160	17.25575
170	25.83219
180	38.63975
190	56.79672
200	79.95747

Remark: Vapor pressure vs temperature data for MHHPA were calculated using PREDICT Version 4.09 software as supplied by Dragon Technologies, Inc. The method employed was that of Pitzer (see Pitzer, K. S., et al.). Pitzer's method of estimation uses the following equation:

$$\text{Log } P_{VR} = P^{(0)} + \omega P^{(1)}$$

Where P_{VR} is the vapor pressure at reduced temperature (temperature/critical temperature), $P^{(0)}$ and $P^{(1)}$ are tabulated functions (see reference) and ω is the accentric factor.

Reference: Pitzer KS, Lippman DZ, Curl, Jr. RF, Huggins CM, Petersen DE. 1955. The Volumetric and Thermodynamic Properties of Fluids. II. Compressibility Factor, Vapor Pressure, and Entropy of Vaporization. J. Am. Chem. Soc., 77, 3433 (1955)

2.5 PARTITION COEFFICIENT

- (e) Preferred result (score = 2)
- | | |
|-----------------|---|
| log P_{ow} : | 2.59 at 25° C |
| Method: | Other (calculated); KOWWIN |
| Year: | |
| GLP: | No |
| Source: | KOWWIN, v1.66 |
| Test Substance: | MHHPA (CAS No. 25550-51-0) |
| Reference: | KOWWIN is part of EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |

*2.6 WATER SOLUBILITY

- (a) Preferred result (score = 1)
- | | |
|------------|---|
| Value: | 4700 to 4820 mg/l of solution at $20.0 \pm 0.5^{\circ}\text{C}$ |
| Remark: | Measured using an adaptation of the flask method, Method 105 of the OECD Guidelines for Testing of Chemicals, 27 July 1995. Due to the rapid hydrolysis of MHHPA, direct application of this method was not possible. Solubility estimated by visual inspection of the presence or absence of test substance in the test systems. |
| Remark: | The quasi-measured aqueous solubility of MHHPA (within 4700 to 4820 mg/l) is within a factor of 12 of the solubility calculated (385 mg/L) using WSKOW v. 1.37 (EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |
| Reference: | Methylhexahydrophthalic Anhydride (MHHPA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/003, 29 May, 2002 |

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

- (a) Preferred value (score = 1c)
- | | |
|-----------------|--|
| Type: | Other; see remarks |
| Light Source: | |
| Light spect.: | |
| Rel. intensity: | based on intensity of sunlight |
| Degradation: | |
| Method: | |
| GLP: | |
| Remark: | Vapor phase Methylhexahydrophthalic Anhydride (MHHPA) is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. MHHPA that becomes associated with water vapor will rapidly hydrolyse to its diacid. The 2 nd order rate constant for reaction with hydroxyl radicals was calculated as 8.51 E-12 cm ³ /(molecule*sec). Based on 1.5E6 OH molecules/cm ³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 30 hours. |
| Reference: | AOPWIN. Version 1.90. Atmospheric Oxidation. EPWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |

3.1.2 STABILITY IN WATER

- (a) Preferred value (score = 1)
- | | |
|------------|--|
| Type | abiotic |
| t1/2 pH7 | <1 day at 25 degrees C |
| t1/2 pH9 | <1 day at 25 degrees C |
| t1/2 pH4 | <1 day at 25 degrees C |
| Method: | calculated |
| Year: | |
| GLP: | no |
| Remark: | No MHHPA was detected at 2.4 hours at 50 degrees C at all pH values tested (pH 4, 7, 9) |
| Remark: | Assessment of hydrolytic stability was carried out using Method 111 of the OECD Guidelines for Testing of Chemicals, 12 May 1981. |
| Reference: | Methylhexahydrophthalic Anhydride (MHHPA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/003, 29 May, 2002 |

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Preferred value	(score = 1c)
Media:	other: air, water, soil, and sediment
Method Calculation:	fugacity model level III
Year:	
Remark:	Air: half-life = 30.2 hr, emissions = 1000 kg/hr Water: half-life = 360 hr, emissions = 1000 kg/hr Soil: half-life = 360 hr, emissions = 1000 kg/hr Sediment: half-life = 1440 hr, emissions = 0 kg/hr Persistence Time: 286 hr
Remark:	Physical properties used as model input parameters were water solubility of 384.5 mg/l, vapor pressure of 0.0332 mm Hg, log Kow of 2.59, and melting point of 5.43°C. All property values were calculated by EPIWIN models.
Remark:	MHHPA is known to rapidly hydrolyze in water to it's diacid. This was not accounted for by EPIWIN calculated water and soil half-lives or the theoretical distribution.
Air:	3.84%
Water:	38.2%
Soil:	57.7%
Sediment:	0.229%
Reference:	Level III Fugacity Model. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.

201-14899B2

Nadic Methyl Anhydride (NMA)

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT**

(a) Preferred result (score = 1)

Value: <-20 degree C

Remark : Measured using BS4633: Method for the Determination of Crystallizing Point, Method 102 of the OECD Guidelines for Testing of Chemicals, 27 July 1995.

Reference: NADIC METHYL ANHYDRIDE (NMA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories
Project Number: 1592/001, 29 May, 2002

***2.2 BOILING POINT**

(a) Preferred result (score = 1)

Value: 277 degrees C

Remark: Measured at 98.75 kPa, by differential scanning calorimetry, using ASTM E537-86, Method 103 of the OECD Guidelines for Testing of Chemicals, 27 July 1995.

Reference: NADIC METHYL ANHYDRIDE (NMA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories
Project Number: 1592/001, 29 May, 2002

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*2.4 VAPOUR PRESSURE

(a) Preferred result (score = 2)

Value: 9.88 E-4 mm Hg

Temperature: 25 degree C

Test substances: NMA

Remark: Calculated using the Pitzer method

Remark:

Temp, degree C	Vapor Pressure mm Hg
25	0.000988
35	0.00266
45	0.00684
55	0.01672
65	0.03724
75	0.0836
85	0.1672
95	0.3192
105	0.6612
115	1.216
125	2.204
135	3.8
145	6.46
155	10.64
165	15.96
175	24.32
185	35.72
195	53.2
205	73.72
215	106.4
225	144.4
235	190
245	258.4
255	334.4
287	760

Remark: Vapor pressure vs temperature data for NMA were calculated using PREDICT Version 4.09 software as supplied by Dragon Technologies, Inc. The method employed was that of Pitzer (see Pitzer, K. S., et al.). Pitzer's method of estimation uses the following equation:

$$\text{Log } P_{VR} = P^{(0)} + \omega P^{(1)}$$

Where P_{VR} is the vapor pressure at reduced temperature (temperature/critical temperature), $P^{(0)}$ and $P^{(1)}$ are tabulated functions (see reference) and ω is the acentric factor.

Reference: Pitzer KS, Lippman DZ, Curl, Jr. RF, Huggins CM, Petersen DE. 1955. The Volumetric and Thermodynamic Properties of Fluids. II. Compressibility Factor, Vapor Pressure, and Entropy of Vaporization. J. Am. Chem. Soc., 77, 3433 (1955)

2.5 PARTITION COEFFICIENT

- (e) Preferred result (score = 2)
- | | |
|-----------------|---|
| log P_{ow} : | 2.27 at 25° C |
| Method: | Other (calculated); KOWWIN |
| Year: | |
| GLP: | No |
| Source: | KOWWIN, v1.66 |
| Test Substance: | NMA (CAS No. 25134-21-8) |
| Reference: | KOWWIN is part of EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |

*2.6 WATER SOLUBILITY

- (a) Preferred result (score = 1)
- | | |
|------------|---|
| Value: | 105 to 146 mg/l at 20 degree C |
| Remark: | Measured using an adaptation of the flask method, Method 105 of the OECD Guidelines for Testing of Chemicals, 27 July 1995. Due to the rapid hydrolysis of NMA, direct application of this method was not possible. Solubility estimated by visual inspection of the presence or absence of test substance in the test systems. |
| Remark: | The quasi-measured aqueous solubility of NMA (within 105 to 146 mg/l) is within a factor of 4 to 6 of the solubility calculated (653 mg/L) using WSKOW v. 1.37 (EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |
| Reference: | NADIC METHYL ANHYDRIDE (NMA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/001, 29 May, 2002. |

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

(a) Preferred value (score = 1c)

Type: Other; see remarks

Light Source:

Light spect.:

Rel. intensity: based on intensity of sunlight

Degradation:

Method:

GLP:

Remark: Vapor phase Nadic Methyl Anhydride (NMA) is susceptible to reaction with photochemically produced hydroxyl (OH) radicals and with ozone (O₃). NMA that becomes associated with water vapor will rapidly hydrolyse to its diacid. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 60.92E-12 cm³/(molecule*sec). Based on 1.5E6 OH molecules/cm³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 4.2 hours. The second order rate for reaction with ozone was calculated as 20.0 E-17 cm³/(molecule*sec). Based on 7.0 E 11 O₃ molecules/cm³, the estimated half-life for reaction with ozone is 1.375 hours. The combined photo-oxidation reaction rate is 1.04 hours.

Reference: AOPWIN. Version 1.90. Atmospheric Oxidation. EPWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.

3.1.2 STABILITY IN WATER

(a)	Preferred value (score = 1)
Type	abiotic
t1/2 pH7	<1 day at 25 degrees C
t1/2 pH9	<1 day at 25 degrees C
t1/2 pH4	<1 day at 25 degrees C
Method:	calculated
Year:	
GLP:	no
Remark:	No NMA was detected at 2.4 hours at 50 degrees C at all pH values tested (pH 4, 7, 9)
Remark:	Assessment of hydrolytic stability was carried out using Method 111 of the OECD Guidelines for Testing of Chemicals, 12 May 1981.
Reference:	NADIC METHYL ANHYDRIDE (NMA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/001, 29 May, 2002.

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Preferred value	(score = 1c)
Media:	other: air, water, soil, and sediment
Method Calculation:	fugacity model level III
Year:	
Remark:	Air: half-life = 1.04 hr, emissions = 1000 kg/hr Water: half-life = 360 hr, emissions = 1000 kg/hr Soil: half-life = 360 hr, emissions = 1000 kg/hr Sediment: half-life = 1440 hr, emissions = 0 kg/hr Persistence Time: 275 hr
Remark:	Physical properties used as model input parameters were water solubility of 653 mg/l, vapor pressure of 0.0151 mm Hg, log Kow of 2.27, and melting point of 26°C. All property values were calculated by EPIWIN models.
Remark:	NMA is known to rapidly hydrolyze in water to it's diacid. This was not accounted for by EPIWIN calculated water and soil half-lives or the theoretical distribution.
Air:	0.192%
Water:	41.7%
Soil:	57.9%
Sediment:	0.166%
Reference:	Level III Fugacity Model. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.

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Hexahydrophthalic Anhydride (HHPA)**2. PHYSICAL-CHEMICAL DATA*****2.4 VAPOUR PRESSURE**

(a) Preferred result (score = 2)

Value: 1.72 E-3

Temperature: 20 degree C

Remark: Calculated using the Pitzer method

Remark:

Temperature degree C	mm Hg
20	0.001721
30	0.004684
40	0.011897
50	0.027988
60	0.06259
70	0.134388
80	0.271844
90	0.516654
100	1.021151
110	1.888203
120	3.330375
130	5.664375
140	9.632848
150	15.09062
160	23.27571
170	34.49927
180	50.89934
190	73.94466
200	103.5302

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Remark: Vapor pressure vs temperature data for HHPA were calculated using PREDICT Version 4.09 software as supplied by Dragon Technologies, Inc. The method employed was that of Pitzer (see Pitzer, K. S., et al.). Pitzer's method of estimation uses the following equation:

$$\text{Log } P_{VR} = P^{(0)} + \omega P^{(1)}$$

Where P_{VR} is the vapor pressure at reduced temperature (temperature/critical temperature), $P^{(0)}$ and $P^{(1)}$ are tabulated functions (see reference) and ω is the accentric factor.

Reference: Pitzer KS, Lippman DZ, Curl, Jr. RF, Huggins CM, Petersen DE. 1955. The Volumetric and Thermodynamic Properties of Fluids. II. Compressibility Factor, Vapor Pressure, and Entropy of Vaporization. J. Am. Chem. Soc., 77, 3433 (1955)

2.5 PARTITION COEFFICIENT

- (e) Preferred result (score = 2)
- | | |
|-----------------|---|
| log P_{ow} : | 2.17 at 25° C |
| Method: | Other (calculated); KOWWIN |
| Year: | |
| GLP: | No |
| Source: | KOWWIN, v1.66 |
| Test Substance: | HPHA (CAS No. 85-42-7) |
| Reference: | KOWWIN is part of EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |

*2.6 WATER SOLUBILITY

- (a) Preferred result (score = 1)
- | | |
|------------|--|
| Value: | 290 to 367 mg/l of solution at $20.0 \pm 0.5^{\circ}\text{C}$ |
| Remark: | Measured using an adaptation of the flask method, Method 105 of the OECD Guidelines for Testing of Chemicals, 27 July 1995. Due to the rapid hydrolysis of HHPA, direct application of this method was not possible. Solubility estimated by visual inspection of the presence or absence of test substance in the test systems. |
| Remark: | The quasi-measured aqueous solubility of HHPA (within 290 to 367 mg/l) differs from the calculated solubility (1,014 mg/L) by a factor of about 3. Solubility of HHPA was calculated using WSKOW v. 1.40 (EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |
| Reference: | Hexahydrophthalic Anhydride (HHPA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/004, 29 May, 2002 |

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

(a)	Preferred value (score = 1c)	
	Type:	Other; see remarks
	Light Source:	
	Light spect.:	
	Rel. intensity:	based on intensity of sunlight
	Degradation:	
	Method:	
	GLP:	
	Remark:	Vapor phase Hexahydrophthalic Anhydride (HHPA) is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. HHPA that becomes associated with water vapor will rapidly hydrolyse to its diacid. The 2 nd order rate constant for reaction with hydroxyl radicals was calculated as 6.82 E-12 cm ³ /(molecule*sec). Based on 1.5E6 OH molecules/cm ³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 37.7 hours.
	Reference:	AOPWIN. Version 1.90. Atmospheric Oxidation. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.

3.1.2 STABILITY IN WATER

(a)	Preferred value (score = 1)	
	Type	abiotic
	t1/2 pH7	<1 day at 25 degrees C
	t1/2 pH9	<1 day at 25 degrees C
	t1/2 pH4	<1 day at 25 degrees C
	Method:	calculated
	Year:	
	GLP:	no
	Remark:	No HHPA was detected at 2.4 hours at 50 degrees C at all pH values tested (pH 4, 7, 9)
	Remark:	Assessment of hydrolytic stability was carried out using Method 111 of the OECD Guidelines for Testing of Chemicals, 12 May 1981.
	Reference:	Hexahydrophthalic Anhydride (HHPA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/004, 29 May, 2002

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Preferred value	(score = 1c)
Media:	other: air, water, soil, and sediment
Method Calculation:	fugacity model level III
Year:	
Remark:	Air: half-life = 37.7 hr, emissions = 1000 kg/hr Water: half-life = 360 hr, emissions = 1000 kg/hr Soil: half-life = 360 hr, emissions = 1000 kg/hr Sediment: half-life = 1440 hr, emissions = 0 kg/hr Persistence Time: 285 hr
Remark:	Physical properties used as model input parameters were water solubility of 1014 mg/l, vapor pressure of 0.0535 mm Hg, log Kow of 2.17, and melting point of -1.82°C. All property values were calculated by EPIWIN models.
Remark:	HHPA is known to rapidly hydrolyze in water to it's diacid. This was not accounted for by EPIWIN calculated water and soil half-lives or the theoretical distribution.
Air:	4.47%
Water:	40.6%
Soil:	54.8%
Sediment:	0.145%
Reference:	Level III Fugacity Model. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.

201-14899 B4

Tetrahydrophthalic Anhydride (THPA)

2. PHYSICAL-CHEMICAL DATA

***2.2 BOILING POINT**

(a) Preferred result (score = 1)

Value: 301 degrees C

Remark: Measured at 101.53 kPa, by differential scanning calorimetry, using ASTM E537-86, Method 103 of the OECD Guidelines for Testing of Chemicals, 27 July 1995.

Reference: TETRAHYDROPHthalic ANHYDRIDE (THPA):
Determination Of General Physico-Chemical Properties,
SafePharm Laboratories Project Number: 1592/002, 29 May, 2002

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*2.4 VAPOUR PRESSURE

(a) Preferred result (score = 2)

Value: 1.32 E-3

Temperature: 20 degree C

Test substances: THPA

Remark: Calculated using the Pitzer method

Remark:

Temperature degree C	mm Hg
20	0.001322
30	0.00365
40	0.00938
50	0.02237
60	0.050299
70	0.108706
80	0.221102
90	0.43857
100	0.81349
110	1.56765
120	2.797977
130	4.789851
140	8.082547
150	13.04705
160	20.2031
170	30.43652
180	44.60361
190	64.97372
200	93.09742

Remark: Vapor pressure vs temperature data for THPA were calculated using PREDICT Version 4.09 software as supplied by Dragon Technologies, Inc. The method employed was that of Pitzer (see Pitzer, K. S., et al.). Pitzer's method of estimation uses the following equation:

$$\text{Log } P_{VR} = P^{(0)} + \omega P^{(1)}$$

Where P_{VR} is the vapor pressure at reduced temperature (temperature/critical temperature), $P^{(0)}$ and $P^{(1)}$ are tabulated functions (see reference) and ω is the acentric factor.

Reference: Pitzer KS, Lippman DZ, Curl, Jr. RF, Huggins CM, Petersen DE. 1955. The Volumetric and Thermodynamic Properties of Fluids. II. Compressibility Factor, Vapor Pressure, and Entropy of Vaporization. J. Am. Chem. Soc., 77, 3433 (1955)

2.5 PARTITION COEFFICIENT

- (a) Preferred result (score = 2)
- | | |
|-----------------|---|
| log P_{ow} : | 1.96 at 25° C |
| Method: | Other (calculated); KOWWIN |
| Year: | |
| GLP: | No |
| Source: | KOWWIN, v1.66 |
| Test Substance: | THPA (CAS No. 85-43-8) |
| Reference: | KOWWIN is part of EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |

*2.6 WATER SOLUBILITY

- (a) Preferred result (score = 1)
- | | |
|------------|--|
| Value: | 303 to 349 mg/l of solution at $20.0 \pm 0.5^{\circ}\text{C}$ |
| Remark: | Measured using an adaptation of the flask method, Method 105 of the OECD Guidelines for Testing of Chemicals, 27 July 1995. Due to the rapid hydrolysis of THPA, direct application of this method was not possible. Solubility estimated by visual inspection of the presence or absence of test substance in the test systems. |
| Remark: | The quasi-measured aqueous solubility of THPA (within 303 to 349 mg/l) is within a factor of 5 of the solubility calculated (1579 mg/L) using WSKOW v. 1.37 (EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. |
| Reference: | TETRAHYDROPHthalic ANHYDRIDE (THPA):
Determination Of General Physico-Chemical Properties,
SafePharm Laboratories Project Number: 1592/002, 29 May, 2002 |

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

- (a) Preferred value (score = 1c)
- Type: Other; see remarks
- Light Source:
- Light spect.:
- Rel. intensity: based on intensity of sunlight
- Degradation:
- Method:
- GLP:
- Remark: Vapor phase Tetrahydrophthalic Anhydride (THPA) is susceptible to reaction with photochemically produced hydroxyl (OH) radicals and with ozone (O₃). THPA that becomes associated with water vapor will rapidly hydrolyse to its diacid. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 59.86E-12 cm³/(molecule*sec). Based on 1.5E6 OH molecules/cm³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 4.2 hours. The second order rate for reaction with ozone was calculated as 20.0 E-17 cm³/(molecule*sec). Based on 7.0 E 11 O₃ molecules/cm³, the estimated half-life for reaction with ozone is 1.375 hours. The combined photo-oxidation reaction rate is 1.04 hours.
- Reference: AOPWIN. Version 1.90. Atmospheric Oxidation. EPWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.

3.1.2 STABILITY IN WATER

(a)	Preferred value (score = 1)
Type	abiotic
t1/2 pH7	<1 day at 25 degrees C
t1/2 pH9	<1 day at 25 degrees C
t1/2 pH4	<1 day at 25 degrees C
Method:	calculated
Year:	
GLP:	no
Remark:	No THPA was detected at 2.4 hours at 50 degrees C at all pH values tested (pH 4, 7, 9)
Remark:	Assessment of hydrolytic stability was carried out using Method 111 of the OECD Guidelines for Testing of Chemicals, 12 May 1981.
Reference:	TETRAHYDROPHthalic ANHYDRIDE (THPA): Determination Of General Physico-Chemical Properties, SafePharm Laboratories Project Number: 1592/002, 29 May, 2002

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Preferred value	(score = 1c)
Media:	other: air, water, soil, and sediment
Method Calculation:	fugacity model level III
Year:	
Remark:	Air: half-life = 1.04 hr, emissions = 1000 kg/hr Water: half-life = 360 hr, emissions = 1000 kg/hr Soil: half-life = 360 hr, emissions = 1000 kg/hr Sediment: half-life = 1440 hr, emissions = 0 kg/hr Persistence Time: 275 hr
Remark:	Physical properties used as model input parameters were water solubility of 1579 mg/l, vapor pressure of 0.0575 mm Hg, log Kow of 1.96, and melting point of -0.74°C. All property values were calculated by EPIWIN models.
Remark:	THPA is known to rapidly hydrolyze in water to it's diacid. This was not accounted for by EPIWIN calculated water and soil half-lives or the theoretical distribution.
Air:	0.205%
Water:	43.9%
Soil:	55.7%
Sediment:	0.127%
Reference:	Level III Fugacity Model. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY.